

Resorcinol
108-46-3 | DTXSID2021238

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.91 | 1.08 | 0.91 | 1.08 | 0.92 | 1.00 |

Model Results

Predicted value: 2.47e-04 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.23e-01

Confidence level: 3.90e-01

Nearest Neighbors from the Training Set

| | | |
|---|--|--|
| <div>Image not found</div> <div>3-Methylaniline</div> <div>Measured: 4.89e-04</div> <div>Predicted: 2.01e-01</div> | <div>Image not found</div> <div>4-Aminophenol</div> <div>Measured: 2.40e-05</div> <div>Predicted: 7.78e-05</div> | <div>Image not found</div> <div>2-Methylbenzothiazole</div> <div>Measured: 3.66e-03</div> <div>Predicted: 2.57e-02</div> |
| <div>Image not found</div> <div>1,2,3,4-Tetrachlorobenzene</div> <div>Measured: 2.25e-06</div> <div>Predicted: 3.76e-02</div> | <div>Image not found</div> <div>3-Pentanone</div> <div>Measured: 2.00e-01</div> <div>Predicted: 29.7</div> | |